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# A mesoscopic mechanical model of the surface tension and some simulation results

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**Abstract.** Drops of mercury do not spread on a surface. A metal paper clip can float on water. These phenomena are macroscopic manifestations of molecular interactions and can be explained in terms of surface tension. In this study, we discuss a simple mesoscopic mechanical model of the surface tension and the results of numerical fluid dynamics simulations implemented on the basis of it. We study the droplet formation without and with gravity when it can drop from a narrow hole like a trickling tap and finally the behaviour of free surface liquid in a vessel. Teachers and students can be able to study the surface tension by using the computer simulation as a “tool” for analysing and discussing the droplet and the liquid behaviour in several different conditions.

## 1. Introduction

Drops of mercury do not spread on a surface. A metal paper clip can float on water. A fluid can flow in a thin tube without the assistance of, or even in opposition to, gravity. All these phenomena are macroscopic manifestations of interactions between fluid molecules and can be explained by using the surface tension concept. Surface phenomena are important not only to physics but also to neighbouring disciplines such as physical chemistry, life and health sciences, and engineering.

There are often obscurities and fallacies in the teaching of surface tension at an elementary level and this is perhaps the reason why the subject is no longer so common in today school curricula [1, 2]. For instance, it has been highlighted [1] that an important question to pose to students when the study of the surface tension is tackled from a mechanical point of view is the following: why is surface tension a force parallel to the interface between two media? After all, it seems obvious that it should be perpendicular to the interface. This question could be very useful in order to activate an authentic understanding of the physical meaning of surface tension.

The explanatory power of one scale of modelling versus another has been widely discussed [3], especially in teaching at secondary or college levels. For example, the kinetic molecular model is of greater use in helping to understand the geometric-kinetic properties of gases — change of volume, diffusion — than the thermo-elastic aspects, which involve the dynamic properties of molecules. However, a microscopic description often proves to be excessively complicated and too difficult to master when, for instance, liquids are analysed. On the other hand, there is often a need to find an alternative to a purely macroscopic description. Sometimes, an explanation at the macroscopic scale is insufficient to satisfy the students, especially when a common conception stands in the way. This is why Besson & Viennot [4] proposed to introduce models at an intermediate scale (i.e. mesoscopic) in the teaching–learning process of some topics. From the viewpoint of the physics researcher, such models are less powerful than the kinetic molecular model, but they may be very useful to introduce some ideas at an early stage, as Miller [3] already recommended. In contrast with their quasi-inexistence in pedagogical research papers, such models are very commonly used in physics, especially in hydrodynamics, or electrodynamics and friction in mechanical systems.



In this sense, the pedagogical introduction of models at this scale is justified not only because they are simpler than molecular models; it is also a question of accustoming students to work with a scale that has its own importance in physics. Moreover, it seems also reasonable to make students aware of the usefulness of passing from one to another of the various levels of description at which to build explanations, in many physic contexts.

When the scale changes it is possible to define three kind of models of surface tension: microscopic, macroscopic and mesoscopic. In the microscopic one (mechanical model) surface tension arises from the intermolecular interactions and thermal effects, while macroscopically it can be understood as a force acting along the interface or an energy per unit surface area, [1] by using a thermodynamics approach [5]. Finally, in the mesoscopic model surface tension can be understood by introducing the effects of forces like the intermolecular interactions although on a bigger scale.

In this paper, we deal with the surface tension from a mechanical point of view with the aim of explaining some properties of liquids due to the surface tension.

A simple mesoscopic mechanical model of the surface tension and the results of numerical fluid dynamics simulations implemented on the basis of it and of the Smoothed Particle Hydrodynamics method [6] are presented. Smoothed Particle Hydrodynamics (SPH) method is a method for obtaining approximate numerical solutions to the equations of fluid dynamics by replacing the fluid with a set of mesoscopic overlapping particles. In this study we simulate the behaviour of a liquid made of several particles and study the dynamics of these particles subjected to some boundary conditions, as for instance fixed walls.

We study the liquid behaviour with respect to the following fundamental phenomena: the bi-dimensional droplet formation by starting from a rectangular geometry without gravity, and with gravity when it can drop from a narrow hole like a trickling tap and the liquid in a vessel. For each of these phenomena the time evolution of the shape of liquid is studied and for a better comparison between our results and the experimental ones a representation of the forces applied to each particle in the liquid is given.

## 2. The physical model

The liquid governing equations in the case of the standard continuum model, written in a Lagrangian framework are [6]

$$\frac{d\rho}{dt} = -\rho \cdot \nabla \cdot \mathbf{u} \quad (1)$$

for the mass conservation, and

$$\frac{d\mathbf{u}}{dt} = -\frac{1}{\rho} \nabla P + \frac{\mu}{\rho} \nabla^2 \mathbf{u} + \mathbf{g} \quad (1)$$

for the momentum, where  $\frac{d}{dt} = \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla$  is the total derivative,  $\mathbf{u}$  is the fluid velocity,  $P$  is the fluid pressure,  $\rho$  is the density,  $\mu$  is the dynamic viscosity and  $\mathbf{g}$  is the gravitational acceleration. It is worth noting that the term  $-\frac{1}{\rho} \nabla P$  in the equation (2) is the pressure force per unit mass.

In our model which is based on SPH method, the liquid is considered to be composed of well-defined mass and size particles while spatial derivatives are found by analytical differentiation of interpolation formula.

The size of these particles depends on the spatial resolution necessary for the phenomenon to be simulated and on the efficiency of calculation. Usually, dimensions of the order of the fraction of the millimetre represent a good agreement between the two requirements mentioned above. The fluid thus discretized results to have both a certain viscosity and a surface tension [7]. However, both values are very small and mostly not easily controllable [7].

In the literature different models of SPH surface tension have been recently discussed [8] and among those, the so called *Inter-particle Force Model* is in our opinion better suitable for didactical purpose.

In this model, forces at mesoscopic or macroscopic scale are defined as those present on a microscopic scale. Attractive forces over a long distance and repulsive ones on short distance between the SPH particles are introduced as they were molecules interacting according to Lennard-Jones potential type [9].

According to this model, the previous equation of momentum for the generic SPH particle  $i$  becomes as reported below:

$$\frac{d\mathbf{u}_i}{dt} = -\frac{1}{\rho_i} \nabla P_i + \frac{\mu_i}{\rho_i} \nabla^2 \mathbf{u}_i + \mathbf{g} + \mathbf{F}_i \quad (2)$$

where  $\mathbf{F}_i$  is the *molecular-like force per unit mass* that we add in the equation (2) to take into account the effect of surface tension in liquids.

The liquid equations are approximated by using the SPH formalism [7]. The advancement in time is obtained by a second order accurate method described in Monaghan [7], which is a variant of the leapfrog scheme.

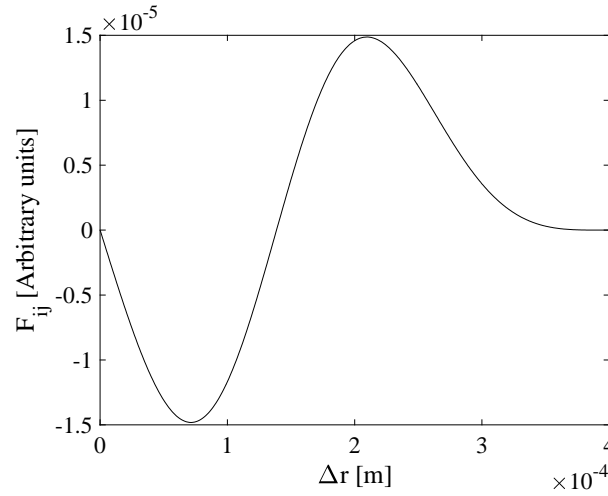
As reported by Tartakowsky and Meakin [9], the exact form of the particle-particle interaction is not critical to the success of the simulations, but it is fundamental that the interactions be repulsive at short distance and attractive at long distances as happens on molecular scale. More details about the role of the repulsive term in the molecular-like force is discussed in the specialised literature [10]. We tested several expressions of forces and we found that the following gave us the best results in terms of correct behaviour of a liquid subjected to a surface tension.

$$\mathbf{F}_{ij} = I_T |\mathbf{r}_{ij}| \left( k - 2e^{-\left(\frac{|\mathbf{r}_{ij}|}{h}\right)^3} \right) W(|\mathbf{r}_{ij}|) \frac{\mathbf{r}_{ij}}{|\mathbf{r}_{ij}|} \quad (3)$$

Equation (4) allow us to calculate the force per unit mass  $\mathbf{F}_{ij}$  on the particle  $i$  due to the particle  $j$ .

$I_T$  is a control parameter to change the intensity of the mesoscopic force and  $k$  is a constant to fix in order to have the maximum positive value of the quantity in equation (4) equal to the minimum negative one. In our study we found that good results were obtained for  $k = 1.434$ .  $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$  is the distance

between two particles. The force is scaled using the function  $W(|\mathbf{r}_i - \mathbf{r}_j|, h)$  (called in the SPH formalism “smoothing kernel”) as a weighting function that has to be continuous and with continuous derivatives over a compact support. In our study we use the polynomial function, called Wendland smoothing kernel, which exhibits very good stability against the tensile instability [11].  $h$  is an important parameter. It is called ‘*smoothing length*’ and controls the interaction size between the particles. The smoothing kernel term gives a contribution in the expression (4) in such a way that the interaction between two particles is repulsive for short distances and attractive over long distances. Following, in the figure 1 the plot of equation (4) for  $k=1.434$  and  $h = 0.2$  mm is sketched.



**Figure 1.** Force  $F_{ij}$  per unit mass on a generic particle  $i$  due to another particle  $j$  as a function of their mutual distance  $\Delta r = |\mathbf{r}_{ij}|$

It represents the force for unit mass between two particles.

The force per unit mass  $\mathbf{F}_i$  on the particle  $i$  due to all other particles is reported below

$$\mathbf{F}_i = \sum_j I_T |\mathbf{r}_{ij}| \left( k - 2e^{-\left(\frac{|\mathbf{r}_{ij}|}{h}\right)^3} \right) \mathbf{W}(|\mathbf{r}_{ij}|) \frac{\mathbf{r}_{ij}}{|\mathbf{r}_{ij}|} \quad (4)$$

Computational efficiency requires a long distance cut-off to reduce the number of particle-particle interactions that must be calculated in the computer simulation. In our case the force is repulsive for distances less than  $2/3h$ , attractive for distances between  $2/3h$  and  $2h$  and zero for distances bigger than  $2h$ . So, the preview force per unit mass calculated by equation (5) has to be considered only to all the particles in the range distance  $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$  equal to  $2h$ .

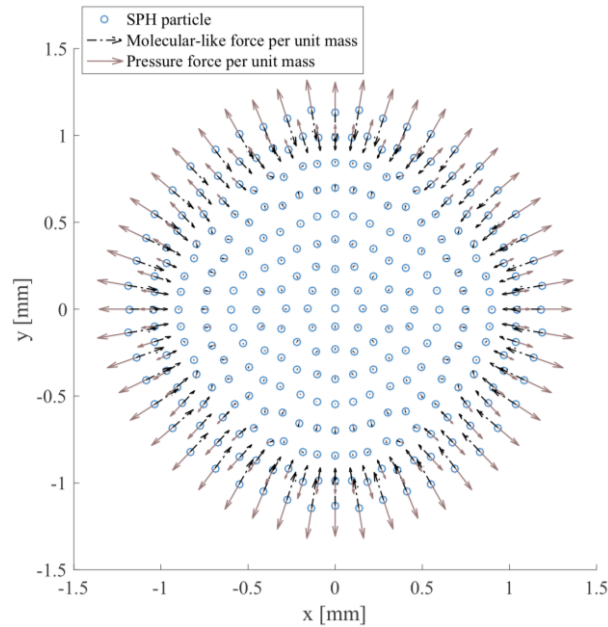
In this study, we consider the liquid slightly compressible because better suited to SPH numerical

method [12, 13], and we model its pressure by using the state equation [12, 13],  $P = \frac{\rho_0 c_0^2}{7} \left[ \left( \frac{\rho}{\rho_0} \right)^7 - 1 \right]$

where the sound speed  $c_0$  is chosen 10 times greater than the maximum speed that a fluid particle can assume. In this way the speed of sound is large enough for the density fluctuation to be negligible [7]. So, in our case  $c_0 = (2ad)^{1/2}$ , where  $d$  is the height of the liquid “slice” and  $a$  is the typical acceleration of the SPH particles.

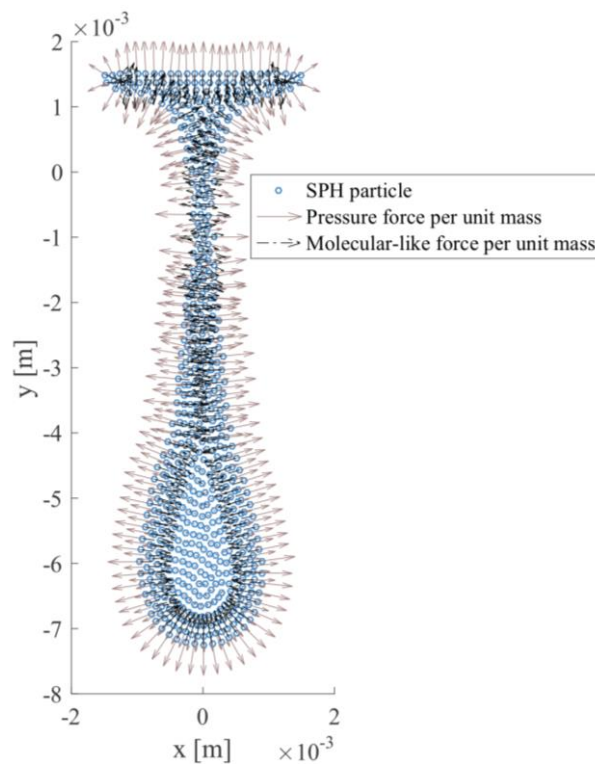
### 3. Simulation results

In figure 2 the simulation results obtained by the implementation on the model described above are shown. We obtained this result after a fairly long simulation time in order to reach the static equilibrium, by starting from a rectangular configuration (far from equilibrium) of the particles without gravity. In this case the value of the parameter  $I_T$  is 3.0. As you can see in figure 2, we obtain a correct circular shape made of SPH particles (like a bi-dimensional drop) and the molecular-like forces per unit mass  $\mathbf{F}_i$  are considerably bigger than zero only on the particles on the edge of the drop. Moreover, on each particle the value of the pressure force per unit mass is equal to the molecular-like force per unit mass  $\mathbf{F}_i$  in order to assure the static equilibrium.



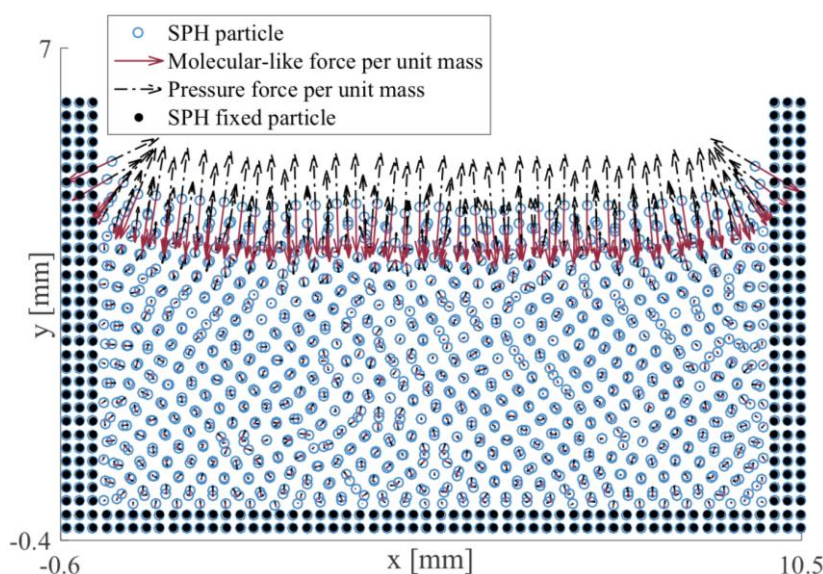
**Figure 2.** Bi-dimensional liquid droplet made of SPH particles at equilibrium for  $h = 0.2$  mm and initial inter-particles distance equal to 0.125 mm. The black dashed arrows are the resultant of the molecular-like forces per unit mass. The brown arrows are the resultant of pressure force per unit mass. The radius of the droplet is  $R = 1.5$  mm

In figure 3 we show the shape of a liquid drop subjected to the gravity after some time steps simulation by starting from a rectangular disposition of the SPH particles. The small layer of particles in the highest region is composed by fixed particles. Also in this case the value of the parameter  $I_T$  is equal to 3.0. In this case there is not static equilibrium.



**Figure 3.** Spatial Distribution of the SPH particles for  $h = 0.2$  mm and initial inter-particles distance equal to 0.125 mm. The black dashed rows are the resultant of the molecular-like forces for unit mass, the brown arrows are the resultant of pressure force for unit mass.

Finally, we simulate a liquid (e.g. water) in a vessel with a value of the parameter  $I_T$  equal to 3.0. The three small layers of particles on the left, on the right and at the bottom regions of the vessel are composed by fixed SPH particles (black dots). In this case the interaction between two liquid particles and between a liquid particle and a fixed particle is almost of equal intensity  $I_T$ . As you can see in figure 4 the meniscus on the left and right borders of the vessel on the free surface of the liquid are clearly shown. Also in this case for each particle the molecular like force per unit mass and the pressure force per unit mass are almost equal and a static equilibrium has been reached.



**Figure 4.** Spatial distribution of the SPH particles at equilibrium for  $h = 0.375$  mm and initial inter-particles distance equal to 0.2 mm. The particles (black dot) on the right, on the left and at the bottom regions are fixed. The red rows are the resultant of the molecular-like forces per unit mass, the black dashed ones are the resultant of pressure forces per unit mass.

#### 4. Conclusions

A very simple mechanical model of the surface tension and some computer simulation results based on it have been presented. Our study discusses the use of an inter-particle force on mesoscopic scale like those usually introduced on a molecular scale. Our model takes into account the internal dynamics of a portion of liquid by the overall effect of the forces applied to each particle composing it and allowed us to study the time evolution of this portion by showing also the shape reached at the equilibrium.

The simulation results based on this model show a correct reproduction of some behaviours like those we observe in real experiments. In order to test our model three different experimental conditions related to three different phenomena involving the surface tension are studied from a numerical point of view. In particular, we discuss the droplet formation by starting from a rectangular geometry of SPH particles with and without gravity. In the first case we observe the correct formation of circular shape. In this second case we observe the behaviour of a liquid that can drop from a narrow hole like a trickling tap. Finally, we show the concave meniscus in a vessel containing a liquid like water.

High school and undergraduate students can explore those phenomena by “playing” with the computer simulation, adjusting some physical fundamental quantities by using the simulation parameters. Teachers and students are allowed to study the surface tension by using the computer simulation as a “tool” for analysing and discussing the behaviour of a portion of liquid in several different conditions.

The results we describe in this paper are still qualitative/semi-quantitative and therefore further studies are needed. Particularly, it is necessary to test the model in other experimental conditions and also to better quantitative correlate the typical quantities of our model with the macroscopic values of the surface tension of different liquids. Moreover, a study aimed at verifying the pedagogical efficacy of the approach here discussed in allowing to the students a better understanding of some experimental results involving capillarity and so on needs to be performed.

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